

3-(6-Methoxy-2-naphthyl)-1-(2-thienyl)-prop-2-en-1-one

H. S. Yathirajan,^a B. Narayana,^b
B. Ashalatha,^b B. K. Sarojini^c and
Michael Bolte^{d*}

^aDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, ^bDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India, ^cDepartment of Chemistry, P. A. College of Engineering, Nadupadavu, Mangalore 574 153, India, and ^dInstitut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail:
bolte@chemie.uni-frankfurt.de

Key indicators

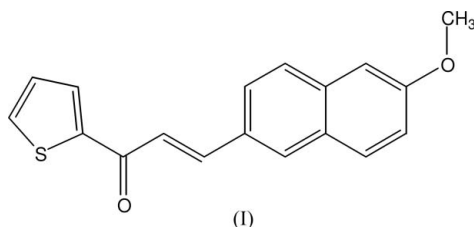
Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.037
 wR factor = 0.102
Data-to-parameter ratio = 13.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The molecule of the title compound, $\text{C}_{18}\text{H}_{14}\text{O}_2\text{S}$, is essentially planar. The central $\text{C}=\text{C}$ double bond is *trans*-configured. Geometric parameters are in normal ranges.

Comment

The title compound, (I), is a biologically active compound. Chalcones and their heterocyclic analogues show various biological effects, *e.g.* anti-inflammatory, antitumour, antibacterial, antitubercular, antiviral, antiprotozoal, gastro-protective *etc.* (Opletalova & Sedivy, 1999). The cytotoxic, anticancer, antiviral, antiprotozoal and insecticidal activities of a variety of chalcones have been reviewed, as well as the enzyme-inhibitory properties and miscellaneous activities of some of these molecules (Dimmock *et al.*, 1999). In addition, with appropriate substituents, chalcones are a class of nonlinear optical (NLO) materials (Fichou *et al.*, 1988; Goto *et al.*, 1991; Butcher *et al.*, 2006; Harrison *et al.*, 2006). The crystal structures of 3-hydroxy-1,3-bis(2-thienyl)prop-2-en-1-one (Baxter *et al.*, 1990), 1,3-bis(4-chlorophenyl)prop-2-en-1-one (Wang *et al.*, 2005), 1-(4-bromophenyl)-3-(2-thienyl)prop-2-en-1-one (Patil *et al.*, 2006) and 1-(4-chlorophenyl)-3-(2-thienyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. In continuation of our work on the crystal structures of chalcones (Yathirajan, Sarojini, Narayana, Ashalatha & Bolte, 2006; Yathirajan, Sarojini, Bindya, Narayana & Bolte, 2006; Yathirajan, Sarojini, Narayana, Bindya & Bolte, 2006), and in view of their importance, we present here the crystal structure of compound (I).



A perspective view of compound (I) is shown in Fig. 1. Bond lengths and angles can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005, updated August 2006; *MOGUL*, Version 1.1; Allen, 2002). The aliphatic double bond is *trans* configured. The molecule is essentially planar (r.m.s. deviation for all non-H atoms is 0.056 Å).

Experimental

Compound (I) was synthesized according to the method reported in the literature (Vogel, 1989) in a yield of 85%. The compound was

Received 28 August 2006
Accepted 4 September 2006

purified by recrystallization from ethanol. Crystal growth was carried out in an acetone–toluene (50:50 v/v) solvent mixture by the slow evaporation technique (m.p. 418–420 K). Analysis for $C_{18}H_{14}O_2S$, found (calculated): C 73.40 (73.44), H 4.75 (4.79)%.

Crystal data

$C_{18}H_{14}O_2S$
 $M_r = 294.35$
 Monoclinic, $P2_1/c$
 $a = 3.9155$ (3) Å
 $b = 10.6776$ (8) Å
 $c = 33.521$ (3) Å
 $\beta = 93.164$ (7)°
 $V = 1399.3$ (2) Å³

$Z = 4$
 $D_x = 1.397$ Mg m^{−3}
 Mo $K\alpha$ radiation
 $\mu = 0.23$ mm^{−1}
 $T = 173$ (2) K
 Rod, yellow
 $0.22 \times 0.12 \times 0.12$ mm

Data collection

Stoe IPDS II two-circle
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (MULABS; Spek, 2003; Blessing,
 1995)
 $T_{\min} = 0.951$, $T_{\max} = 0.970$

10698 measured reflections
 2641 independent reflections
 2315 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.043$
 $\theta_{\max} = 25.7^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.102$
 $S = 1.05$
 2641 reflections
 192 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0685P)^2 + 0.1527P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.28$ e Å^{−3}
 $\Delta\rho_{\min} = -0.34$ e Å^{−3}
 Extinction correction: SHELXL97
 (Sheldrick, 1997)
 Extinction coefficient: 0.036 (5)

H atoms were found in a difference map but they were subsequently refined using a riding model, with C–H = 0.95 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$, or C–H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$. The methyl group was allowed to rotate but not to tip.

Data collection: X-Area (Stoe & Cie, 2001); cell refinement: X-Area; data reduction: X-Area; program(s) used to solve structure: SHELXS97 (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXL97.

BKS thanks the AICTE, Government of India, for financial assistance through the Career Award for Young Teachers Scheme.

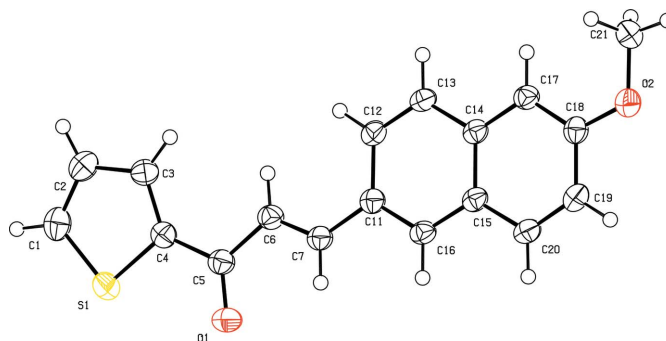


Figure 1

The molecular structure of the title compound, with the atom numbering; displacement ellipsoids are drawn at the 50% probability level.

References

- Allen, F. H. (2002). *Acta Cryst.* **B58**, 380–388.
 Baxter, L. A. M., Blake, A. J., Heath, G. A. & Stephenson, T. A. (1990). *Acta Cryst.* **C46**, 508–510.
 Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
 Butcher, R. J., Yathirajan, H. S., Anilkumar, H. G., Sarojini, B. K. & Narayana, B. (2006). *Acta Cryst.* **E62**, o1659–o1661.
 Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. M. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
 Fichou, D., Watanabe, T., Takeda, T., Miyata, S., Goto, Y. & Nakayama, M. (1988). *Jpn J. Appl. Phys.* **27**, L429–L430.
 Goto, Y., Hayashi, A., Kimura, Y. & Nakayama, M. (1991). *J. Cryst. Growth*, **108**, 688–698.
 Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Indira, J. (2006). *Acta Cryst.* **E62**, o1647–o1649.
 Ng, S.-L., Patil, P. S., Razak, I. A., Fun, H.-K. & Dharmaparakash, S. M. (2006). *Acta Cryst.* **E62**, o3200–o3202.
 Opletalova, V. & Sedivy, D. (1999). *Ceska Slov. Farm.* **48**, 252–255.
 Patil, P. S., Ng, S.-L., Razak, I. A., Fun, H.-K. & Dharmaparakash, S. M. (2006). *Acta Cryst.* **E62**, o3718–o3720.
 Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Stoe & Cie (2001). *X-Area*. Stoe & Cie, Darmstadt, Germany.
 Vogel (1989). *Vogel's Text book of Practical Organic Chemistry*, edited by B. S. Furniss, A. J. Hannaford, P. W. G. Smith & A. R. Tatchell, 5th edition, p. 1034. London: Longman Group UK Ltd.
 Wang, L., Yang, W. & Zhang, D.-C. (2005). *Acta Cryst.* **E61**, o2820–o2822.
 Yathirajan, H. S., Sarojini, B. K., Bindya, S., Narayana, B. & Bolte, M. (2006). *Acta Cryst.* **E62**, o4046–o4047.
 Yathirajan, H. S., Sarojini, B. K., Narayana, B., Ashalatha, B. V. & Bolte, M. (2006). *Acta Cryst.* **E62**, o3964–o3965.
 Yathirajan, H. S., Sarojini, B. K., Narayana, B., Bindya, S. & Bolte, M. (2006). *Acta Cryst.* **E62**, o4048–o4049.